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Centre Borelli - ENS Paris Saclay
Université Paris-Saclay

Journées scientifiques 2024 RT Terre et Energie
November, 7th, 2024



ANR RhoSuNN

(Partially-)saturated granular media.



Macroscopic, non-brownian entities
Stokes flow

Rheology.

Rheology : ” the branch of physics concerned with the flow and change of shape of matter ”

[Collins English Dictionary]

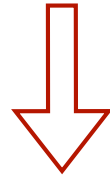
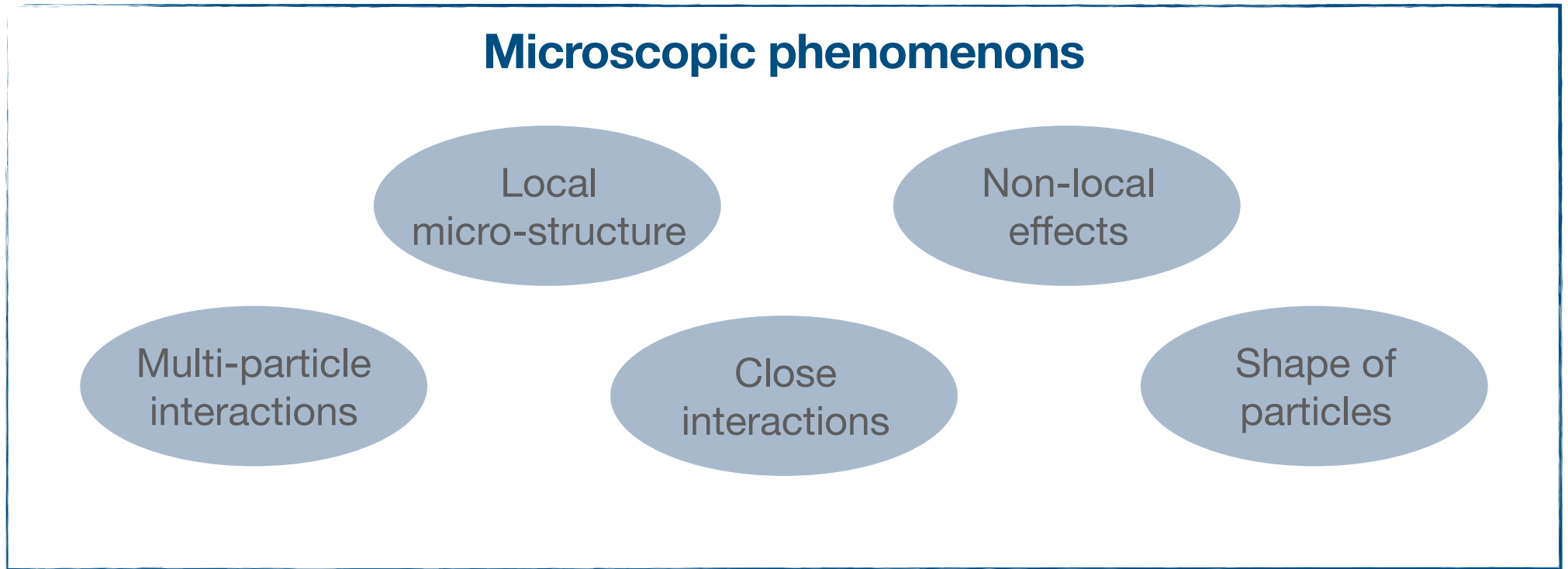
▶ flow, segregation, mixing, blocking, collapse...

Macroscopic behavior

Methodology

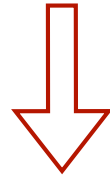
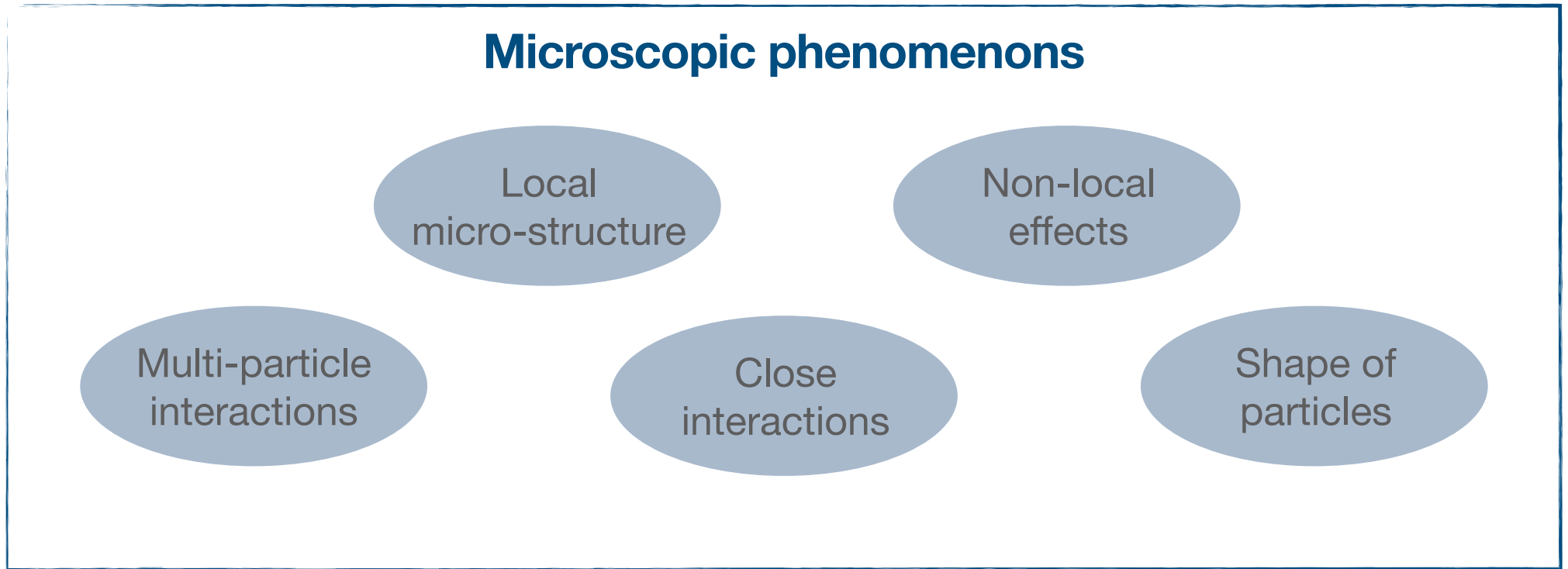
Macroscopic behavior

Methodology



Macroscopic behavior

Methodology

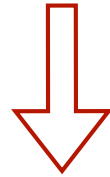
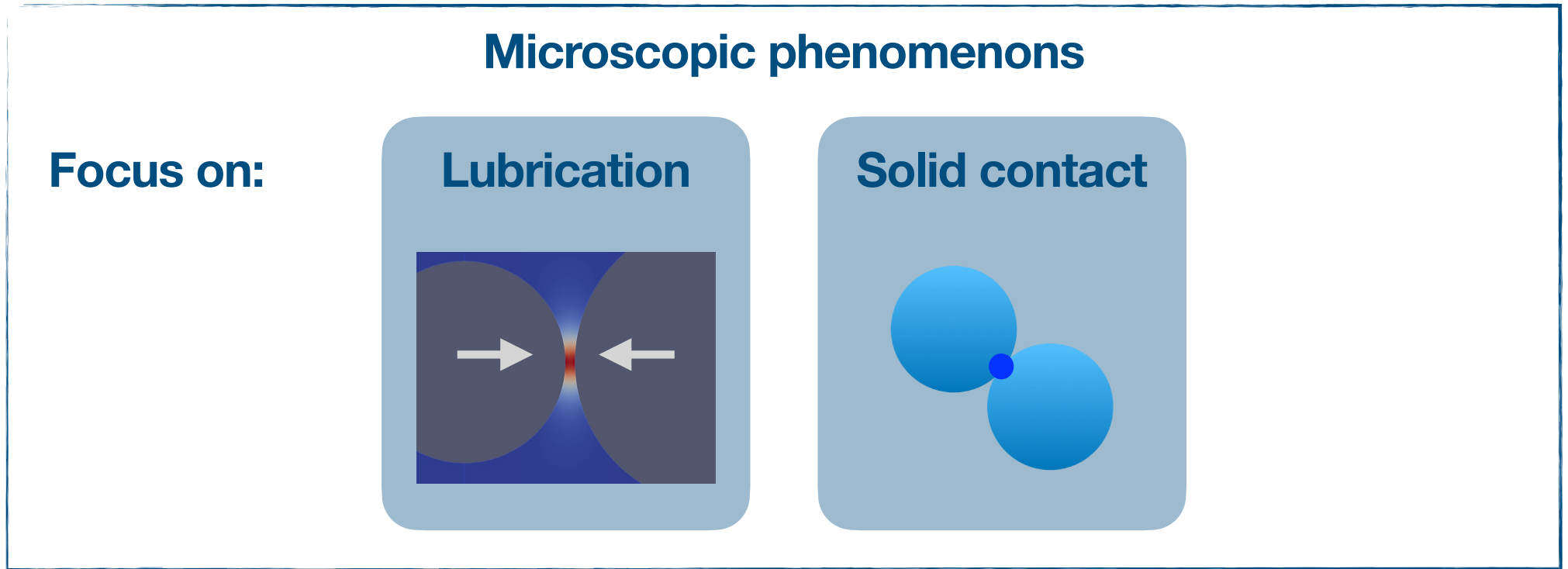


Macroscopic behavior



Numerical simulations at the microscopic level

Methodology



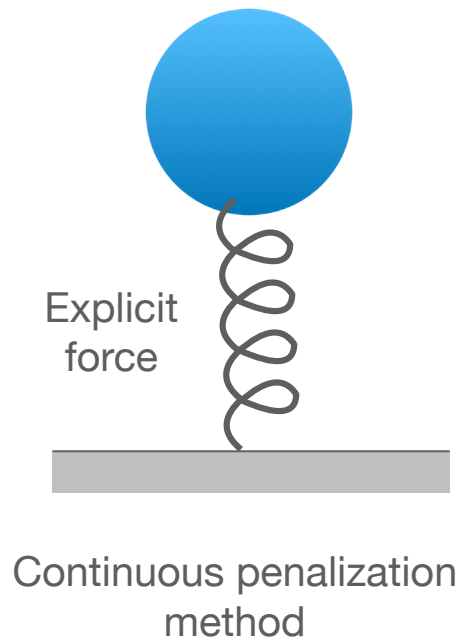
Macroscopic behavior



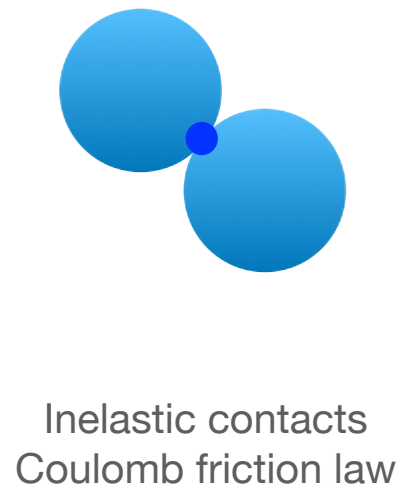
Numerical simulations at the microscopic level

Two class of models.

Explicit penalty force

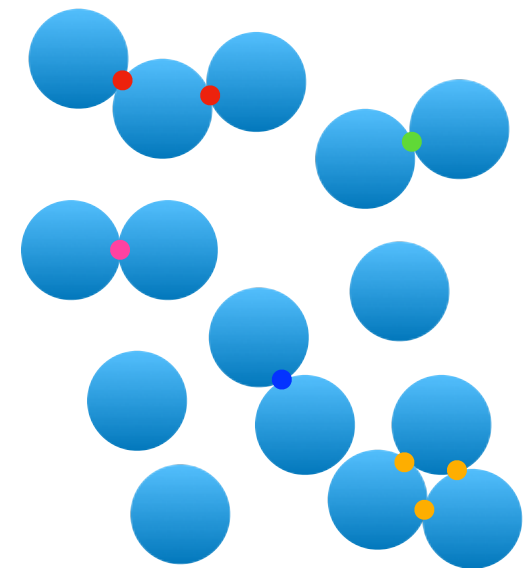


Contact law



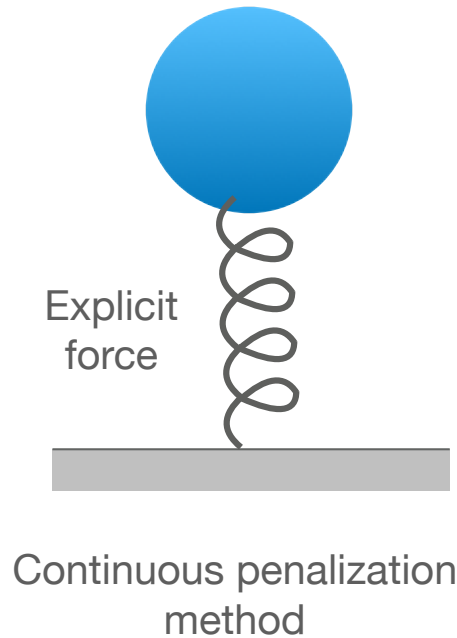
Explicit solution for 2 particles

Multi-contact problem



Two class of models.

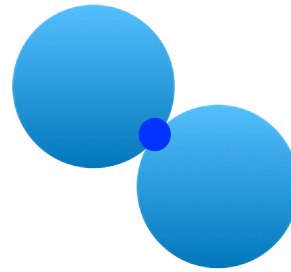
Explicit penalty force



DEM / Molecular Dynamics

[Cundall, Strack, 1979]

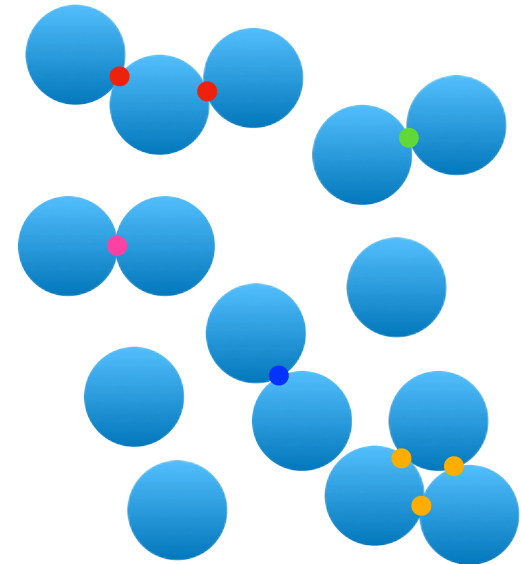
Contact law



Inelastic contacts
Coulomb friction law

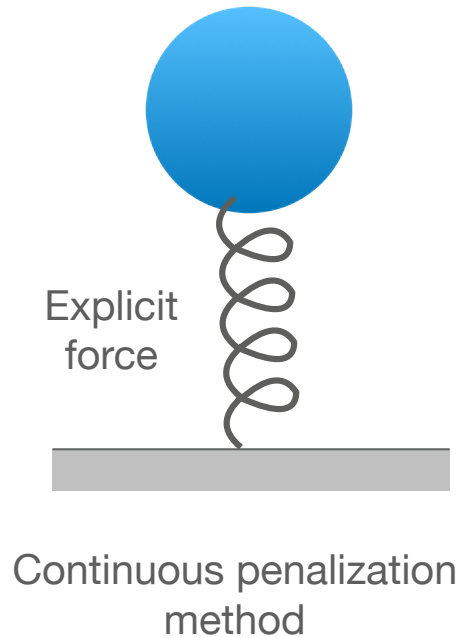
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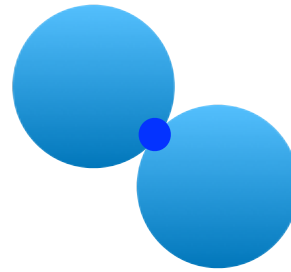
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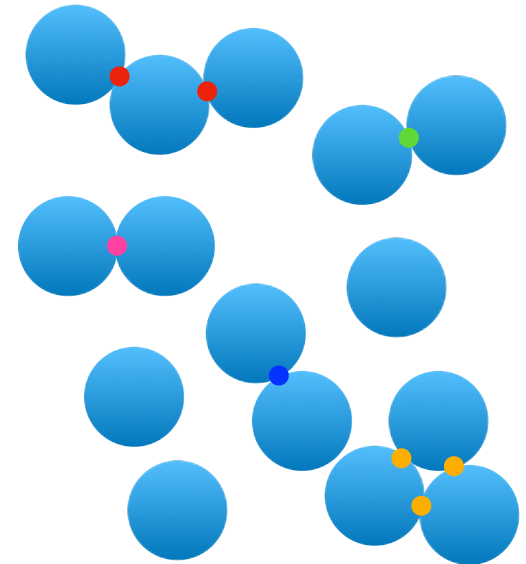
Inelastic contacts
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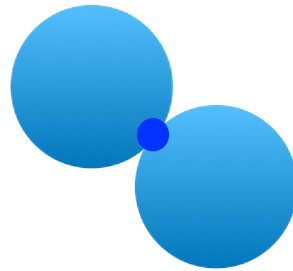
Non-Smooth Contact Dynamics

[Moreau, 1988] [Moreau, Jean, 1992]

Multi-contact problem

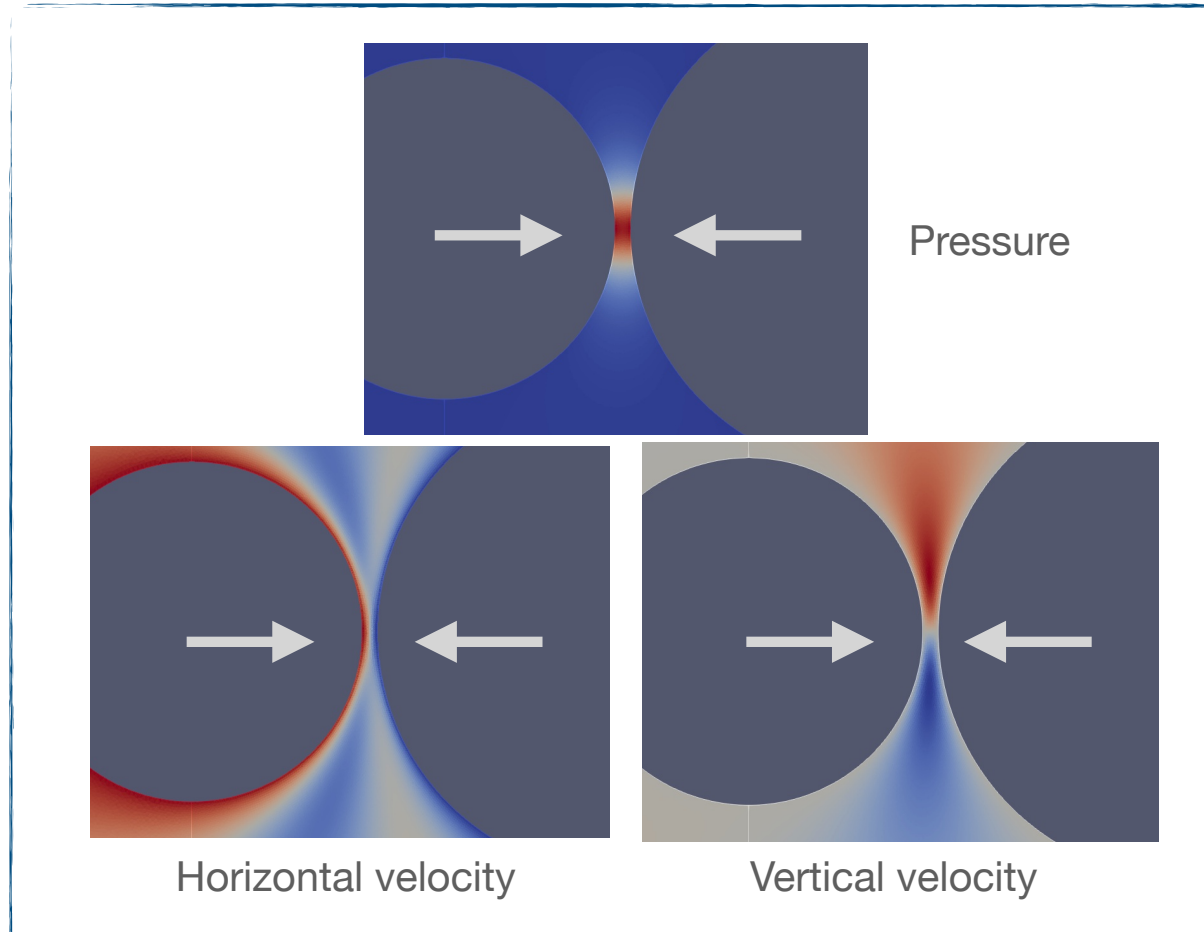


Contact law

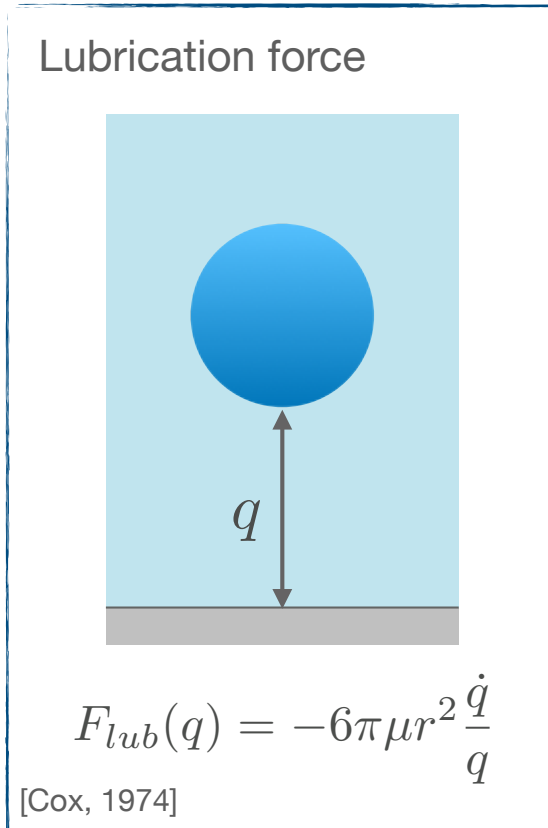


Gluey contact model

Lubrication and Numerical simulations.



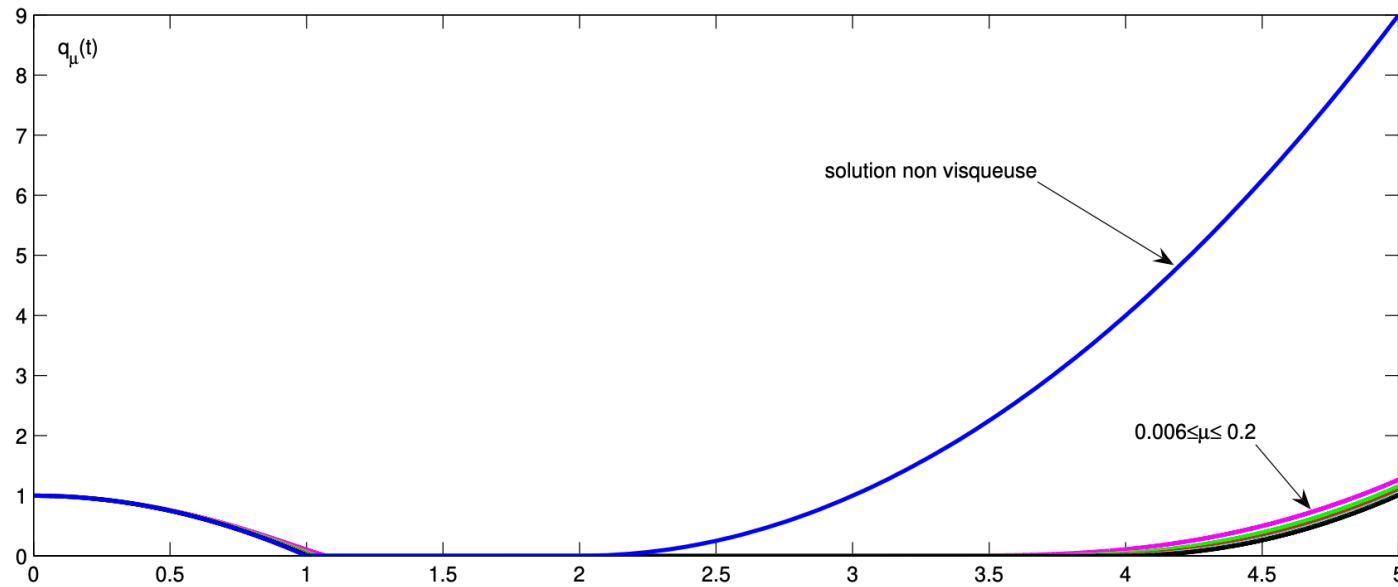
A stiff problem.



$$m\ddot{q} = -6\pi\mu r^2 \frac{\dot{q}}{q} + m f^{\text{ext}}$$

- $q(t) > 0$ for any t
- BUT very small...

Modeling lubrication: the gluey contact model.

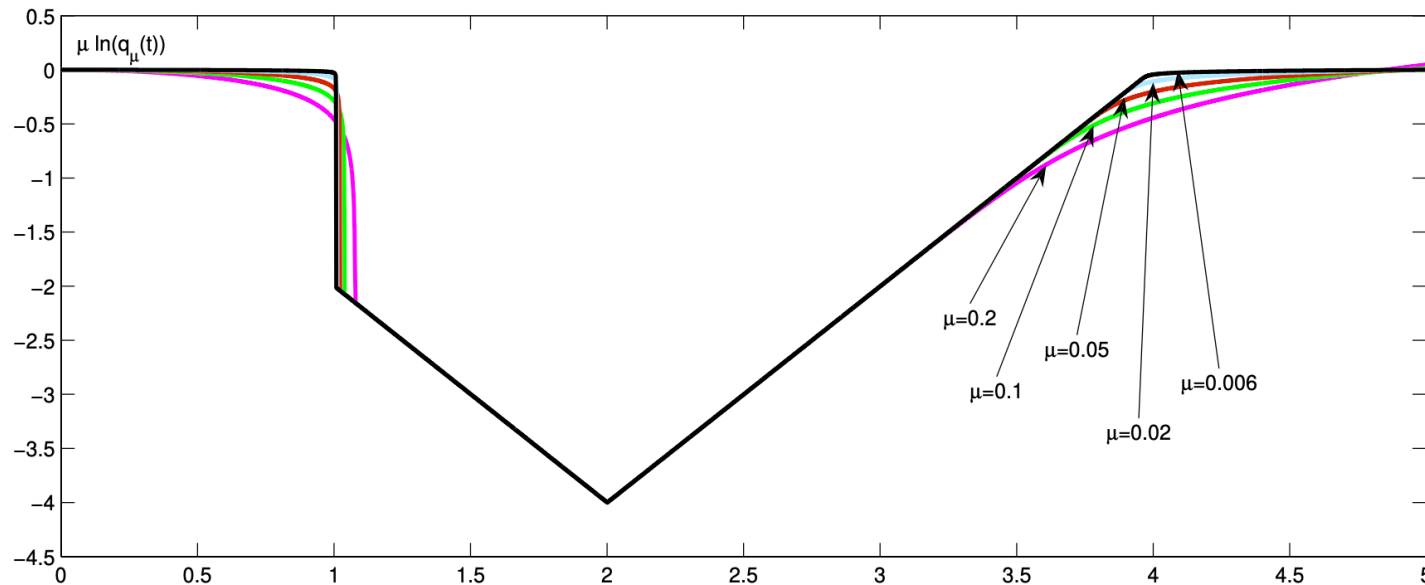


$$f^{\text{ext}} = -2 \mathbf{1}_{[0,2]} + 2 \mathbf{1}_{[2,+\infty]}$$

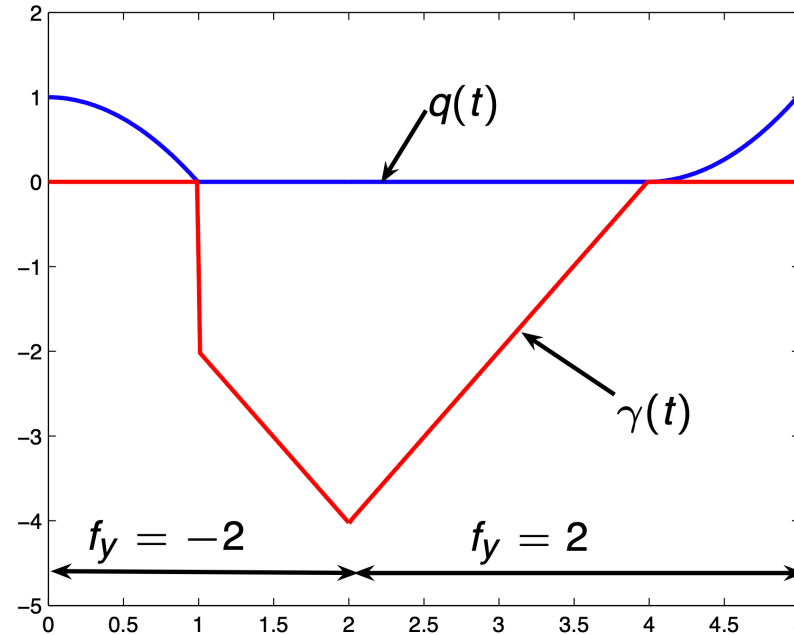
$$\ddot{q}_\mu = -\mu \frac{\dot{q}_\mu}{q_\mu} + f^{\text{ext}}$$

$$\dot{q}_\mu(0) = 0$$

$$q_\mu(0) = 1$$



Modeling lubrication: the gluey contact model.



$$\dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

$$m\ddot{q} = m f^{\text{ext}} + \lambda_n$$

$$\text{supp}(\lambda_n) \subset \{t, q(t) = 0\}$$

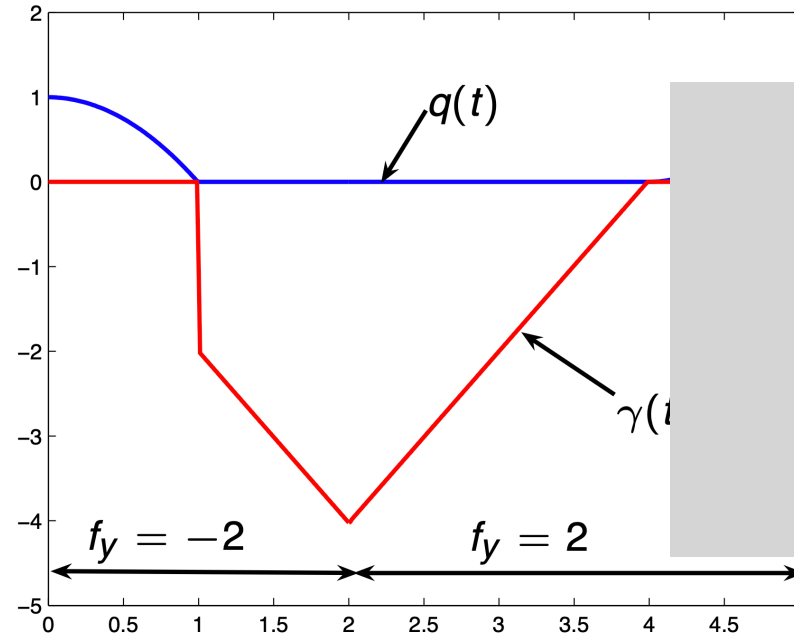
$$\dot{\gamma} = -\lambda_n$$

$$q \geq 0, \gamma \leq 0$$

$$C_{q,\gamma} = \begin{cases} \{0\} & \text{si } \gamma^- < 0 \\ \mathbb{R}^+ & \text{si } \gamma^- = 0 \\ & q = 0 \\ \mathbb{R} & \text{sinon} \end{cases}$$

- B. Maury, A gluey particle model, ESAIM Proceedings, July 2007, Vol.18, 133-142
- A. Lefebvre, Numerical simulation of gluey particles, M2AN, 43:53-80 (2009)

Modeling lubrication: the gluey contact model.



$$\dot{q}^+ = PC_{q,\gamma} \dot{q}^-$$

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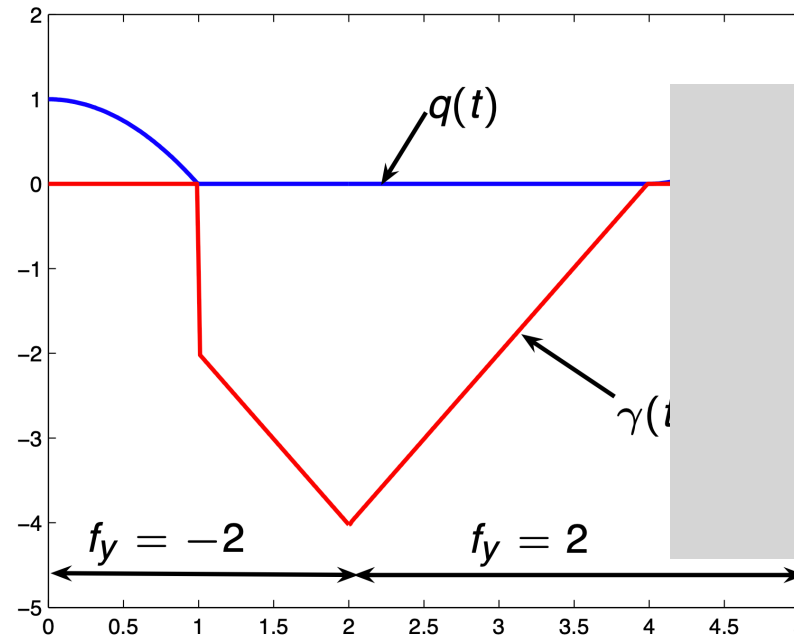
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Modeling lubrication: the gluey contact model.



$$\dot{q}^+ = P_{\mathbb{R}^+} \dot{q}^- = 0$$

$$\dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

$$m\ddot{q} = m f^{\text{ext}} + \lambda_n$$

$$\text{supp}(\lambda_n) \subset \{t, q(t) = 0\}$$

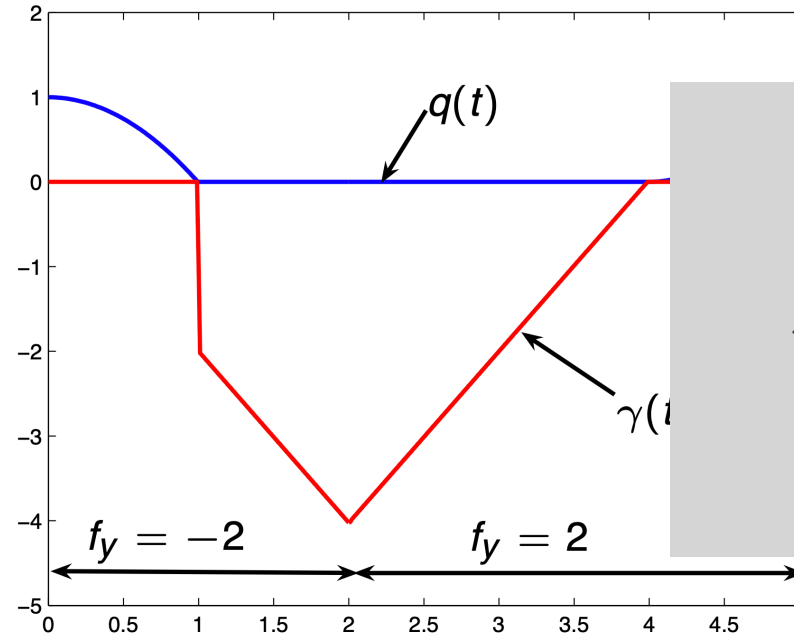
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Modeling lubrication: the gluey contact model.



$$\dot{q}^+ = P_{\mathbb{R}^+} \dot{q}^- = 0$$

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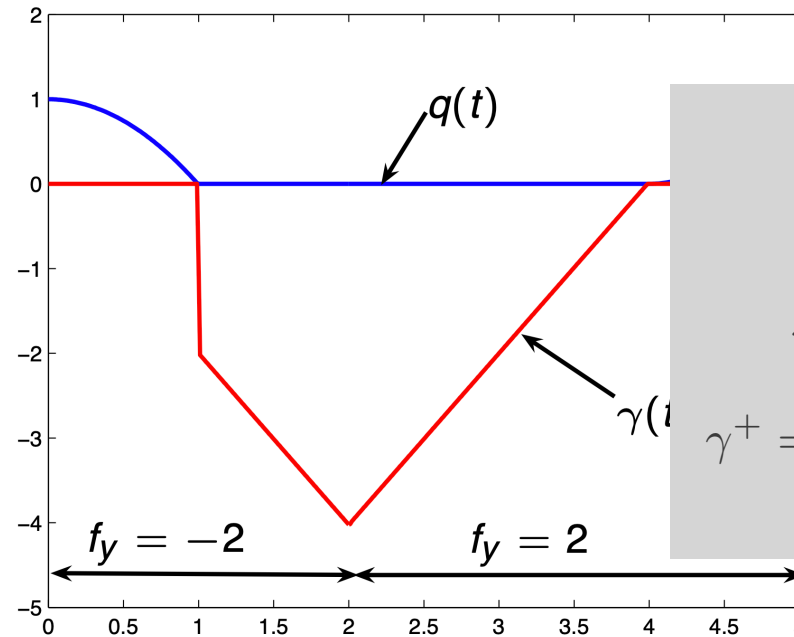
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Modeling lubrication: the gluey contact model.



$$\dot{q}^+ = P_{\mathbb{R}^+} \dot{q}^- = 0$$

$$\lambda_n = m(\dot{q}^+ - \dot{q}^-) = -m\dot{q}^-$$

$$\gamma^+ = \gamma^+ - \gamma^- = -\lambda_n = m\dot{q}^- < 0$$

$$\dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

$$m\ddot{q} = m f^{\text{ext}} + \lambda_n$$

$$\text{supp}(\lambda_n) \subset \{t, q(t) = 0\}$$

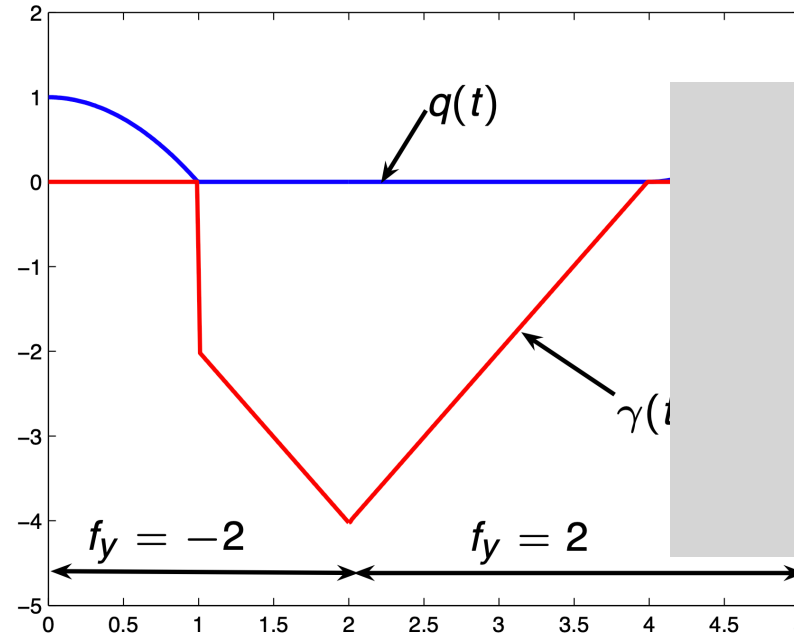
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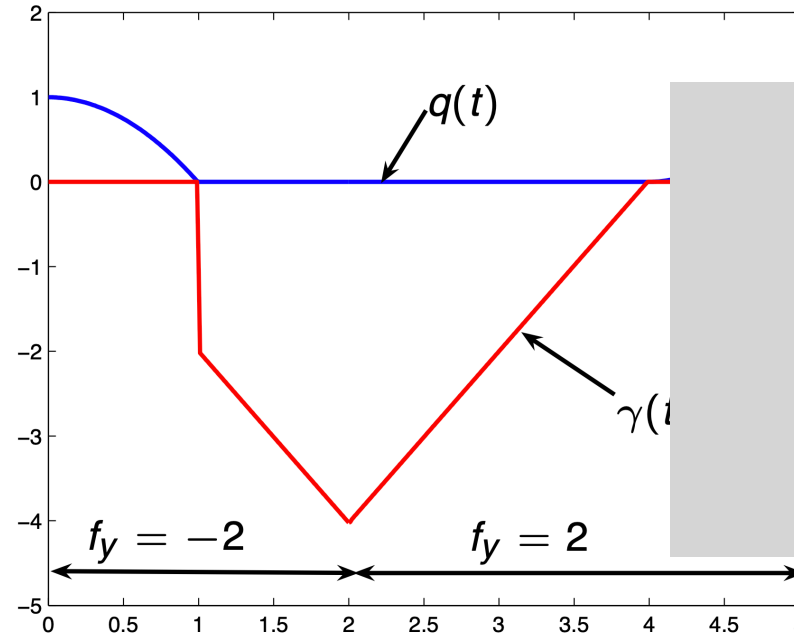
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Modeling lubrication: the gluey contact model.



$$\gamma < 0 \Rightarrow q \equiv 0$$

$$\lambda_n = -m f^{\text{ext}}$$

$$\dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

$$m\ddot{q} = m f^{\text{ext}} + \lambda_n$$

$$\text{supp}(\lambda_n) \subset \{t, q(t) = 0\}$$

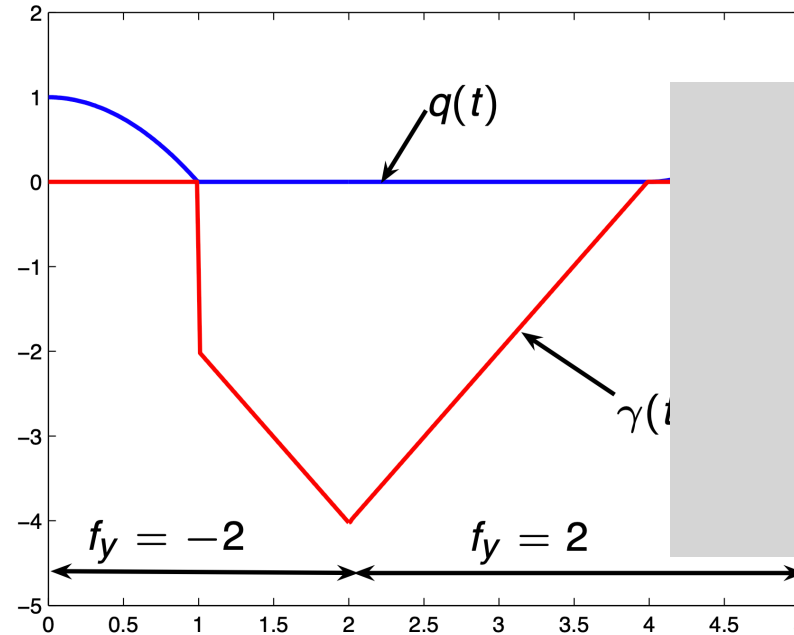
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$$\begin{aligned} \gamma < 0 &\Rightarrow q \equiv 0 \\ \lambda_n &= -m f^{\text{ext}} \\ \dot{\gamma} &= -\lambda_n = m f^{\text{ext}} \end{aligned}$$

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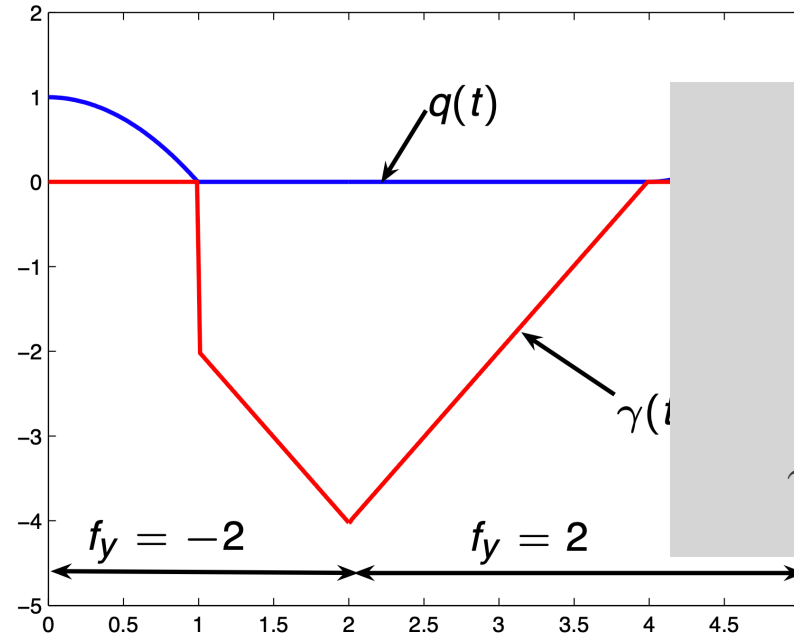
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Modeling lubrication: the gluey contact model.



$$\begin{aligned} \gamma < 0 &\Rightarrow q \equiv 0 \\ \lambda_n &= -m f^{\text{ext}} \\ \dot{\gamma} &= -\lambda_n = m f^{\text{ext}} \\ \gamma(t) &= m \dot{q}^-(t_c) + \int_{t_c}^t m f^{\text{ext}} \end{aligned}$$

$$\dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

$$m \ddot{q} = m f^{\text{ext}} + \lambda_n$$

$$\text{supp}(\lambda_n) \subset \{t, q(t) = 0\}$$

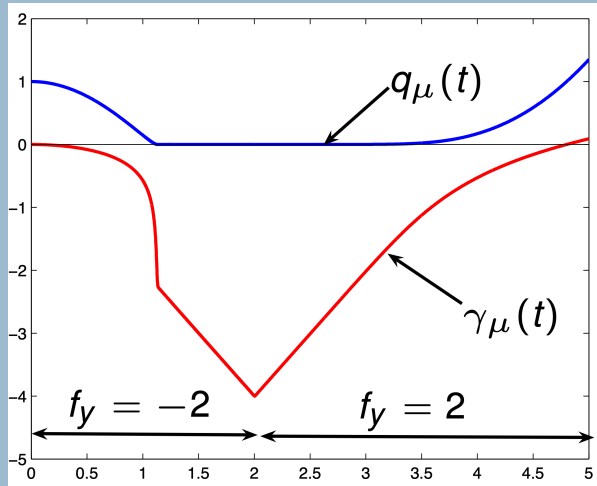
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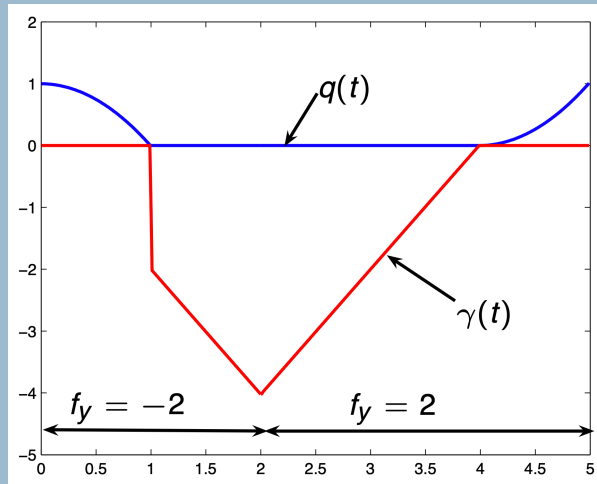
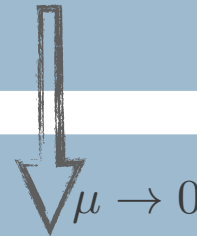
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Convergence result: first order equations.



$$m\dot{q}_\mu(t) + \gamma_\mu(t) = m\dot{q}(0) + \gamma_\mu(0) + m \int_0^t f^{\text{ext}}(s) ds$$

$$\gamma_\mu(t) = \mu \ln(q_\mu(t))$$



$$m\dot{q}(t) + \gamma(t) = m\dot{q}(0) + m \int_0^t f^{\text{ext}}(s) ds$$

$$q \geq 0, \quad \gamma \leq 0, \quad q\gamma = 0$$

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Numerical scheme

$$\text{Contact law: } \dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

► Fully implicit algorithms

$$\bar{u}^{k+1} = u^k + \Delta t f^{\text{ext},k+1}$$

$$u^{k+1} = P_{m,C_{q^k}}(\bar{u}^{k+1})$$

- **Implicit** admissible velocity space

$$C_{q^k} = \{v \in \mathbb{R} / q^{k+1} = q^k + \Delta t v \geq 0$$

$$q^{k+1} = q^k + \Delta t v \leq 0, \quad \gamma^k < 0\}$$

- Anitescu, M., & Hart, G. D. (2004). A constraint-stabilized time-stepping approach for rigid multibody dynamics with joints, contact and friction. *International Journal for Numerical Methods in Engineering*, 60(14), 2335-2371.
- B. Maury. A time-stepping scheme for inelastic collisions. *Numerische Mathematik*, 102(4):649–679, 2006.
- A. Lefebvre, Numerical simulation of gluey particles, M2AN, 43:53-80 (2009)

Numerical scheme

► Fully implicit algorithms

$$\bar{u}^{k+1} = u^k + \Delta t f^{\text{ext},k+1}$$

$$u^{k+1} = P_{m, C_{q^k}}(\bar{u}^{k+1})$$

$$\begin{cases} u \in K \\ J(u) = \min_{v \in K} J(v) \end{cases}$$

Primal problem

Convex
constrained
optimization

- **Implicit** admissible velocity space

$$C_{q^k} = \left\{ v \in \mathbb{R} \mid \begin{aligned} q^{k+1} &= q^k + \Delta t v \geq 0 \\ q^{k+1} &= q^k + \Delta t v \leq 0, \quad \gamma^k < 0 \end{aligned} \right\}$$

Numerical scheme

$$\nabla J(u) = -\lambda \nabla g(u)$$

$$g(u) \leq 0, \quad \lambda \geq 0$$

$$g(u)\lambda = 0$$

Optimality conditions

► Fully implicit algorithms - Convergence result

Model

$$\dot{q}^+ = P_{C_{q,\gamma}} \dot{q}^-$$

$$m\ddot{q} = m f^{\text{ext}} + \lambda_n$$

$$q \geq 0$$

$$\text{supp}(\lambda_n) \subset \{t, q(t) = 0\}$$

$$\dot{\gamma} = -\lambda_n, \quad \gamma \leq 0$$

Algorithm

$$u^{k+1} = P_{m, C_{q^k}}(\bar{u}^{k+1})$$

$$m \frac{u^{k+1} - u^k}{\Delta t} = f^{\text{ext}}(t^k, q^k) + \lambda_+^{k+1} - \lambda_-^{k+1}$$

$$q^k + \Delta t u^{k+1} \geq 0, \quad \lambda_+^{k+1} \geq 0, \quad \lambda_-^{k+1} \geq 0$$

$$(q^k + \Delta t u^{k+1}) \lambda_+^{k+1} = 0$$

$$(q^k + \Delta t u^{k+1}) \lambda_-^{k+1} = 0$$

$$\gamma^{k+1} = \min(0, \gamma^k - \Delta t \lambda^{k+1})$$

Numerical scheme

► Fully implicit algorithms - Dual problem

$$\left| \begin{array}{l} \lambda \in F \\ E(\lambda) = \min_{\mu \in F} E(\mu) \end{array} \right.$$

Dual problem

$$\left| \begin{array}{l} (\lambda_+, \lambda_-) \in F \\ E(\lambda_+, \lambda_-) = \min_{(\mu_+, \mu_-) \in F} E(\mu_+, \mu_-) \end{array} \right.$$

$$F = \mathbb{R}^+ \times \mathbb{R}^+$$

$$E(\mu_+, \mu_-) = (\mu_+ - \mu_-) \left(q^k + \Delta t \frac{u_\mu + \bar{u}^{k+1}}{2} \right)$$

Discrete energy

where
$$m \frac{u_\mu - u^k}{\Delta t} = f^{\text{ext}}(t^k, q^k) + \mu_+ - \mu_-$$

- On convex numerical schemes for inelastic contacts with friction, with H. Bloch, ESAIM:Proc 75 (2023), pp. 24-59
- M. Frémond. Non-Smooth Thermomechanics. Springer Berlin Heidelberg, Berlin, Heidelberg, 2002

$$E(\mu) = \mu \left(\frac{u^+ + u^-}{2} \right)$$

Numerical scheme

► Fully implicit algorithms - Dual problem

$$\left| \begin{array}{l} \lambda \in F \\ E(\lambda) = \min_{\mu \in F} E(\mu) \end{array} \right.$$

Dual problem

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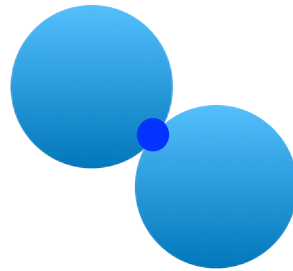
Discrete energy

► Can be solved using Projected Gradient Algorithms

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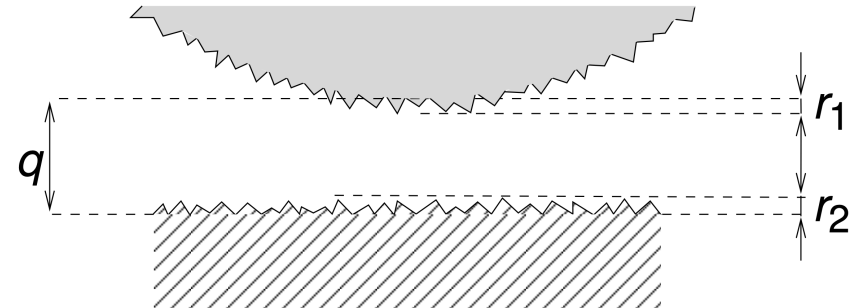
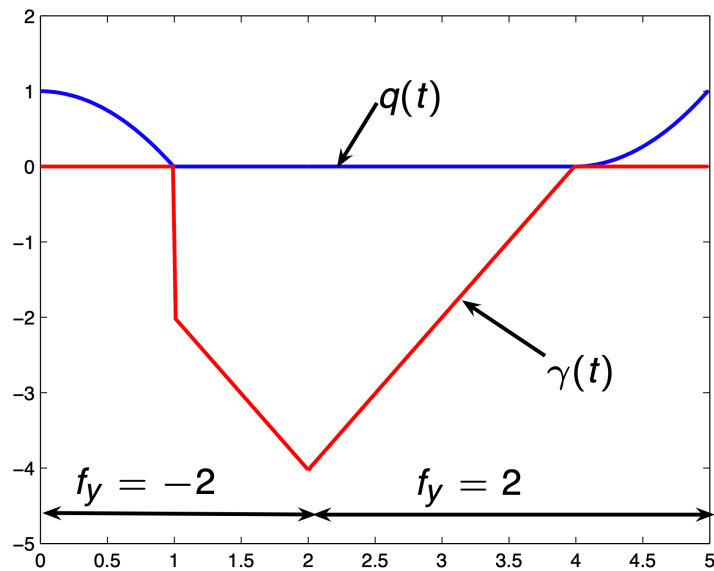
Contact law



Gluey contact model
with inelastic contact

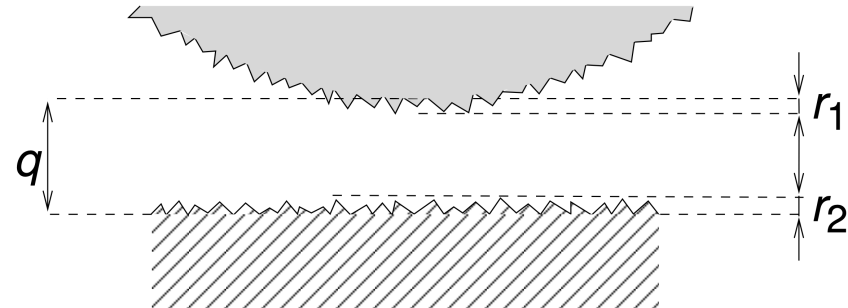
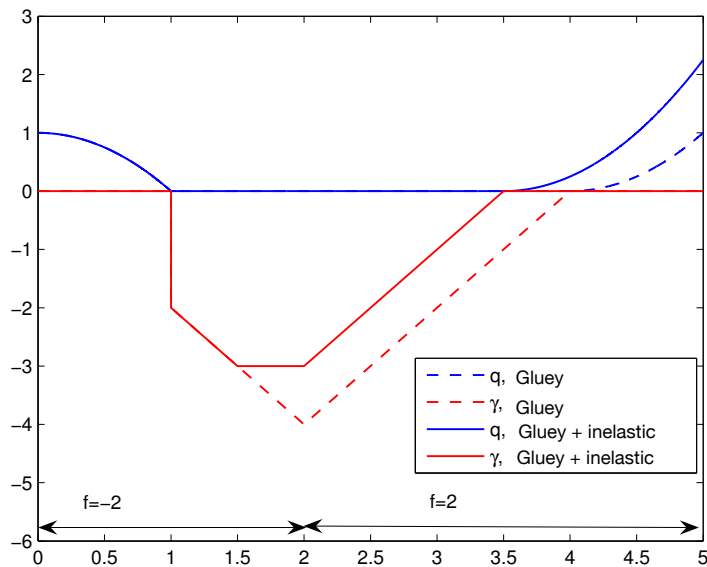
[PhD Quentin Houssier]

Accounting for solid contact



- Roughness \implies contact
- Model : solid contact for $q = r_1 + r_2$

Accounting for solid contact



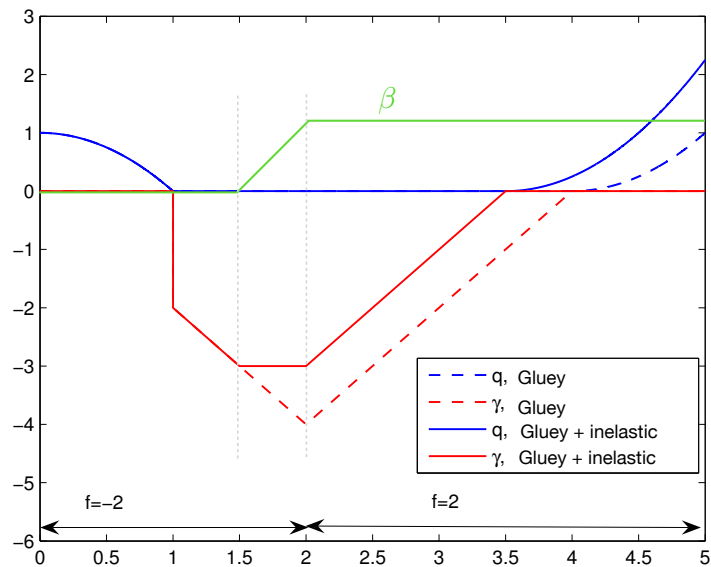
- Roughness \implies contact
- Model : solid contact for $q = r_1 + r_2$

$$\gamma \approx \gamma_\mu(t) = \mu \ln(q_\mu(t))$$

$$\implies \text{Threshold for } \gamma : \gamma \geq \gamma^* = \mu \ln(r_1 + r_2)$$

\implies Easy to implement!

Accounting for solid contact



Model

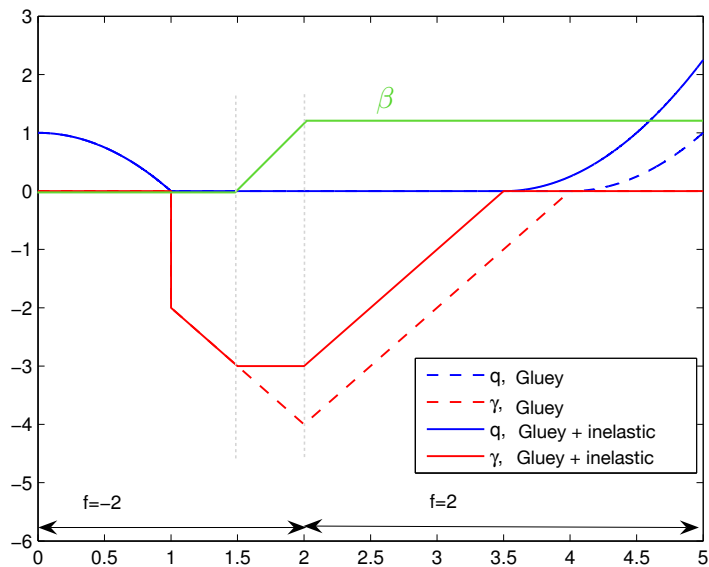
$$m\dot{q}(t) + \gamma(t) + \beta(t) = m\dot{q}(0) + m \int_0^t f^{\text{ext}}(s) ds$$

$$q \geq 0, \quad \gamma \leq 0, \quad q\gamma = 0$$

$$\gamma \geq \gamma^*, \quad \dot{\beta} \geq 0$$

$$\text{supp}(\dot{\beta}) \subset \{t, \gamma(t^+) = \gamma^*\}$$

Accounting for solid contact



- Regularity issues
- Convergence of the numerical scheme
- Existence of solutions

Model

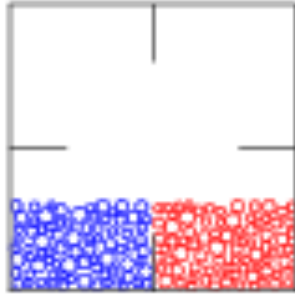
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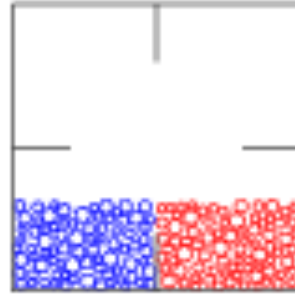
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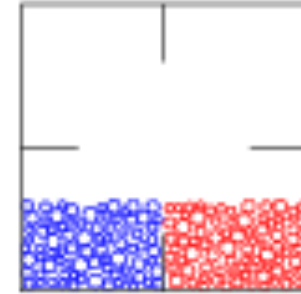
Accounting for solid contact



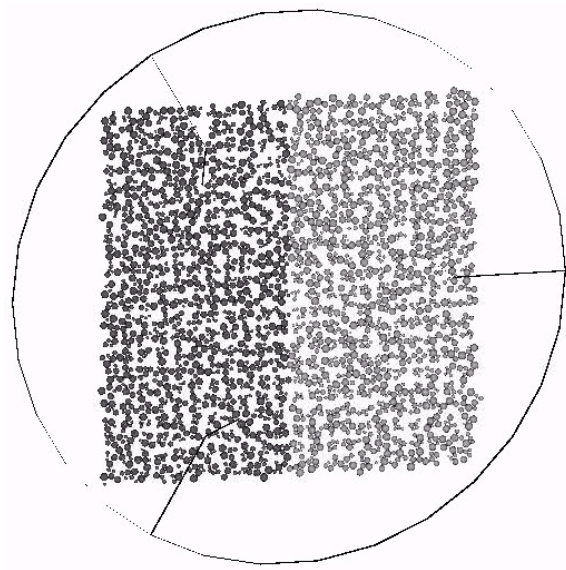
Inelastic contact



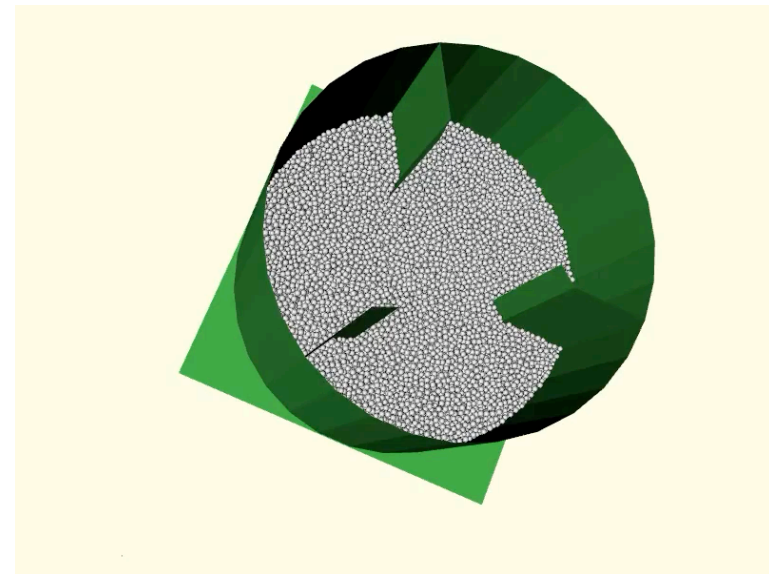
Gluey + Inelastic contact



Gluey contact

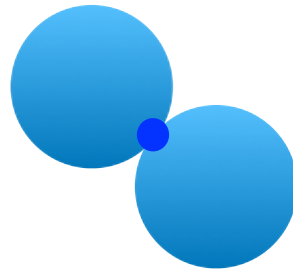


Gluey + Inelastic contact



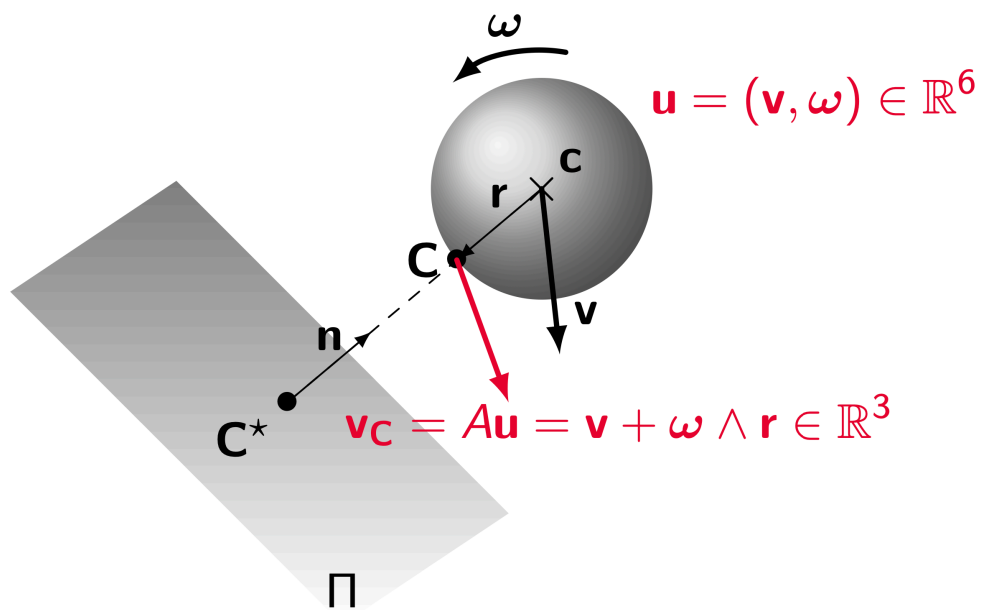
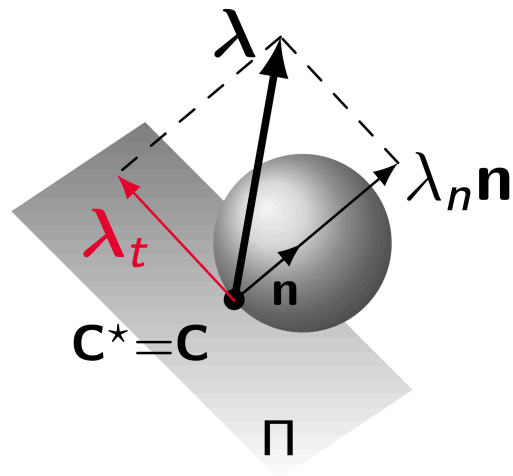
Gluey + Inelastic contact

Contact law



Inelastic contacts
Coulomb friction law

Modeling friction.



► Contact force

$$\boldsymbol{\lambda} = \lambda_n \mathbf{n} + \boldsymbol{\lambda}_t \in \mathbb{R}^3$$

► If $T\mathbf{v}_C^+ = 0$ (no slip)

$$|\boldsymbol{\lambda}_t| \leq \mu \lambda_n$$

► If $T\mathbf{v}_C^+ \neq 0$ (sliding motion)

$$\boldsymbol{\lambda}_t = -\mu \lambda_n \frac{T\mathbf{v}_C^+}{|T\mathbf{v}_C^+|}$$

Modeling friction.

$$M \frac{d\mathbf{u}}{dt} = \mathbf{f}^{\text{ext}} + A^T (\lambda_n \mathbf{n} + \boldsymbol{\lambda}_t) \quad (\text{FPD})$$

$$D(\mathbf{c}) \geq 0, \quad \lambda_n \geq 0, \quad D(\mathbf{c})\lambda_n = 0 \quad (\text{Norm. Cont.})$$

$$\mathbf{u}^+ = P_{C_c} \mathbf{u}^-$$

$$\text{If } \mathbf{T}A\mathbf{u}^+ = 0 \text{ (no slip), } |\boldsymbol{\lambda}_t| \leq \mu\lambda_n \quad (\text{Tang. Cont.})$$

$$\text{If } \mathbf{T}A\mathbf{u}^+ \neq 0 \text{ (sliding motion), } \boldsymbol{\lambda}_t = -\mu\lambda_n \frac{\mathbf{T}\mathbf{v}_C^+}{|\mathbf{T}\mathbf{v}_C^+|}$$

$$[\mathbf{u} = (\mathbf{v}, \boldsymbol{\omega}), \quad A\mathbf{u} = \mathbf{v} + \boldsymbol{\omega} \wedge \mathbf{r}, \quad A^T \boldsymbol{\lambda} = (\boldsymbol{\lambda}, \mathbf{r} \wedge \boldsymbol{\lambda}) \in \mathbb{R}^6]$$

Founding NSCD algorithms

$$M \frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = \mathbf{f}^e + A^{k,T} (\lambda_n \mathbf{n}^k + \boldsymbol{\lambda}_t) \quad (\text{FPD})$$

$$\lambda_n \geq 0 \quad (\text{Norm. Cont.})$$

$$D^k + \Delta t \nabla D^k \cdot \mathbf{v}^{k+1} \geq 0$$

$$(D^k + \Delta t \nabla D^k \cdot \mathbf{v}^{k+1}) \lambda_n = 0$$

$$\text{If } \mathbf{T}^k A^k \mathbf{u}^{k+1} = 0 \quad |\boldsymbol{\lambda}_t| \leq \mu \lambda_n \quad (\text{Tang. Cont.})$$

$$\text{If } \mathbf{T}^k A^k \mathbf{u}^{k+1} \neq 0 \quad \boldsymbol{\lambda}_t = -\mu \lambda_n \frac{\mathbf{T}^k A^k \mathbf{u}^{k+1}}{|\mathbf{T}^k A^k \mathbf{u}^{k+1}|}$$

- Jean, M. (1999). The non-smooth contact dynamics method. *Computer methods in applied mechanics and engineering*, 177(3-4), 235-257.
- Dubois, F., & Jean, M. (2006). The non smooth contact dynamic method: recent LMG90 software developments and application. *Analysis and simulation of contact problems*, 375-378.

Founding NSCD algorithms

Non-convex
problem

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Convex optimization for friction?

$$\left| \begin{array}{l} \lambda \in F \\ E(\lambda) = \min_{\mu \in F} E(\mu) \end{array} \right.$$

Dual problem

$$\left| \begin{array}{l} \lambda \in \mathbf{F} \\ E(\lambda) = \min_{\mu \in \mathbf{F}} E(\mu) \end{array} \right.$$

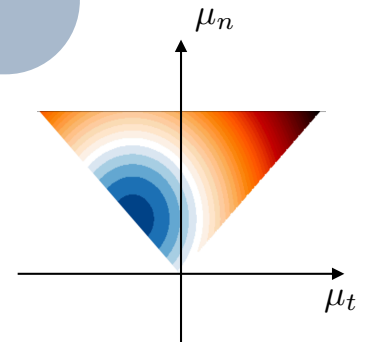
$$\mathbf{F} = \{ \boldsymbol{\mu} = \mu_n \mathbf{n} + \boldsymbol{\mu}_t \in \mathbb{R}^3 \mid |\boldsymbol{\mu}_t| \leq \mu \mu_n \}$$

$$E(\boldsymbol{\mu}) = \mu_n \left[D^k + \Delta t \mathbf{n} \cdot A^k \left(\frac{\mathbf{u}_\mu + \bar{\mathbf{u}}^{k+1}}{2} \right) \right] \\ + \boldsymbol{\mu}_t \cdot \left[\Delta t \mathbf{T}^k A^k \left(\frac{\mathbf{u}_\mu + \bar{\mathbf{u}}^{k+1}}{2} \right) \right]$$

Discrete energy

► Can be solved using Projected Gradient Algorithms

- On convex numerical schemes for inelastic contacts with friction, with H. Bloch, ESAIM:Proc 75 (2023), pp. 24-59
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Convex optimization for friction?

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Dual problem

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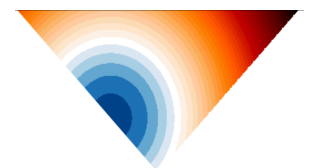
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Discrete energy

Non derivable



► Can be solved using Projected Gradient Algorithms



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Convex optimization for friction?

$$\nabla J(u) \in -\lambda \partial g[u]$$

$$g(u) \leq 0, \quad \lambda \geq 0$$

$$g(u)\lambda = 0$$

Optimality conditions



$$M \frac{\mathbf{u}^{k+1} - \mathbf{u}^k}{\Delta t} = \mathbf{f}^e + A^{k,T} (\lambda_n \mathbf{n}^k + \boldsymbol{\lambda}_t) \quad (\text{FPD})$$

$$\lambda_n \geq 0 \quad (\text{Norm. Cont.})$$

$$D^k + \Delta t \nabla D^k \cdot \mathbf{v}^{k+1} \geq \mu \Delta t |\mathbf{T}^k A^k \mathbf{u}^{k+1}|$$

$$(D^k + \Delta t \nabla D^k \cdot \mathbf{v}^{k+1} - \mu \Delta t |\mathbf{T}^k A^k \mathbf{u}^{k+1}|) \lambda_n = 0$$

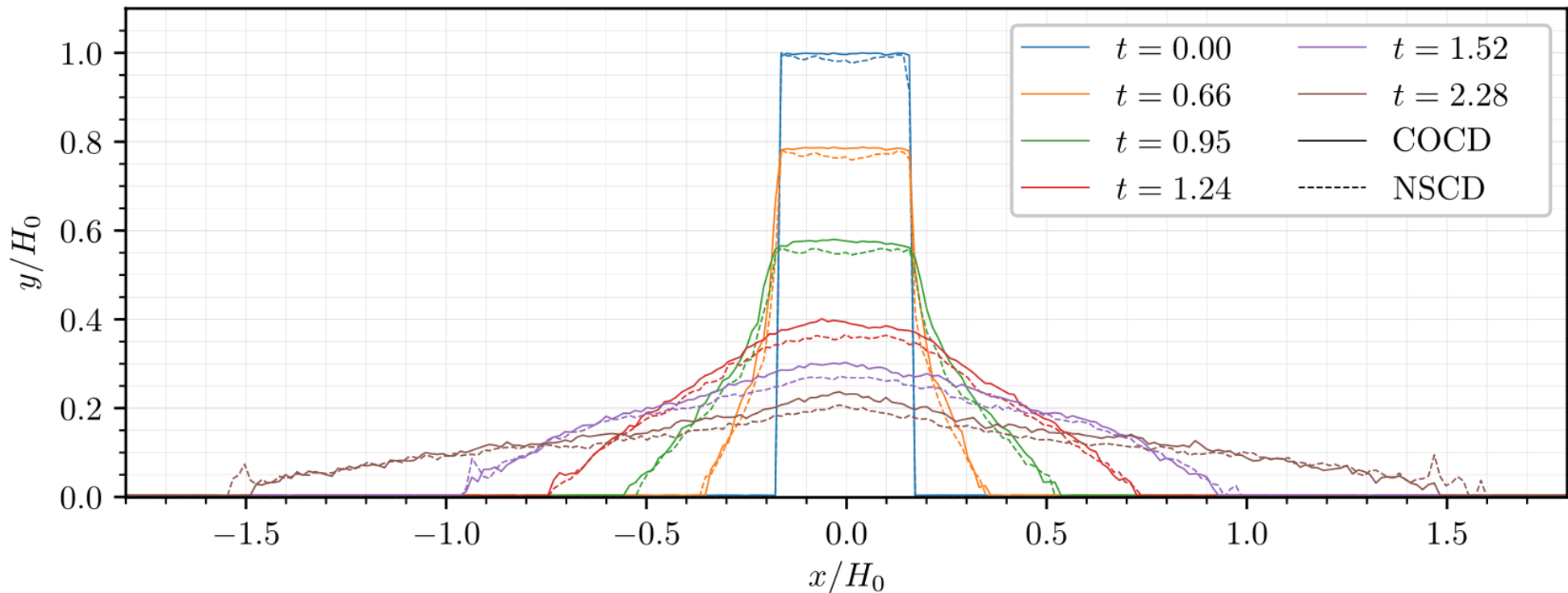
$$\text{If } \mathbf{T}^k A^k \mathbf{u}^{k+1} = 0 \quad |\boldsymbol{\lambda}_t| \leq \mu \lambda_n \quad (\text{Tang. Cont.})$$

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Numerical tests.

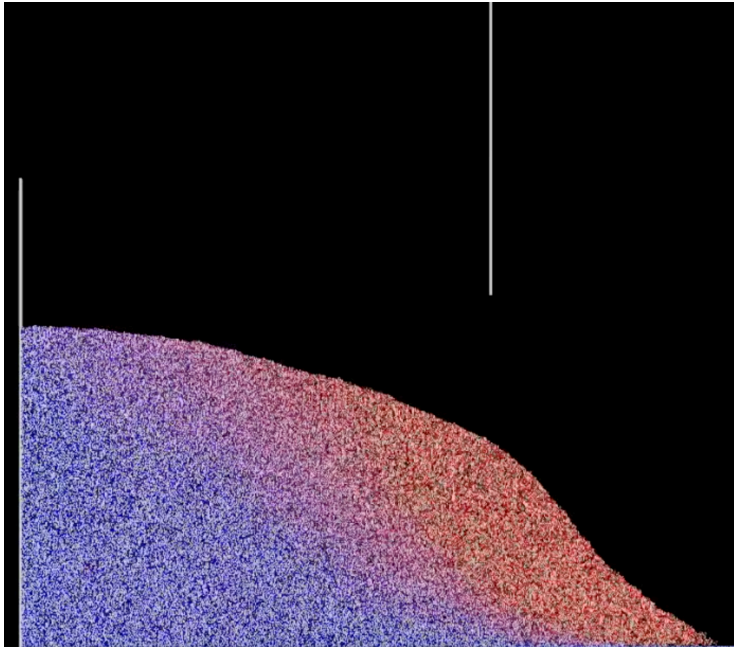
- ▶ PhD Hugo Martin [LJLL, IPGP]
with Y. Maday, A. Mangeney, B. Maury
- ▶ Influence of convexification?

Granular column collapse:

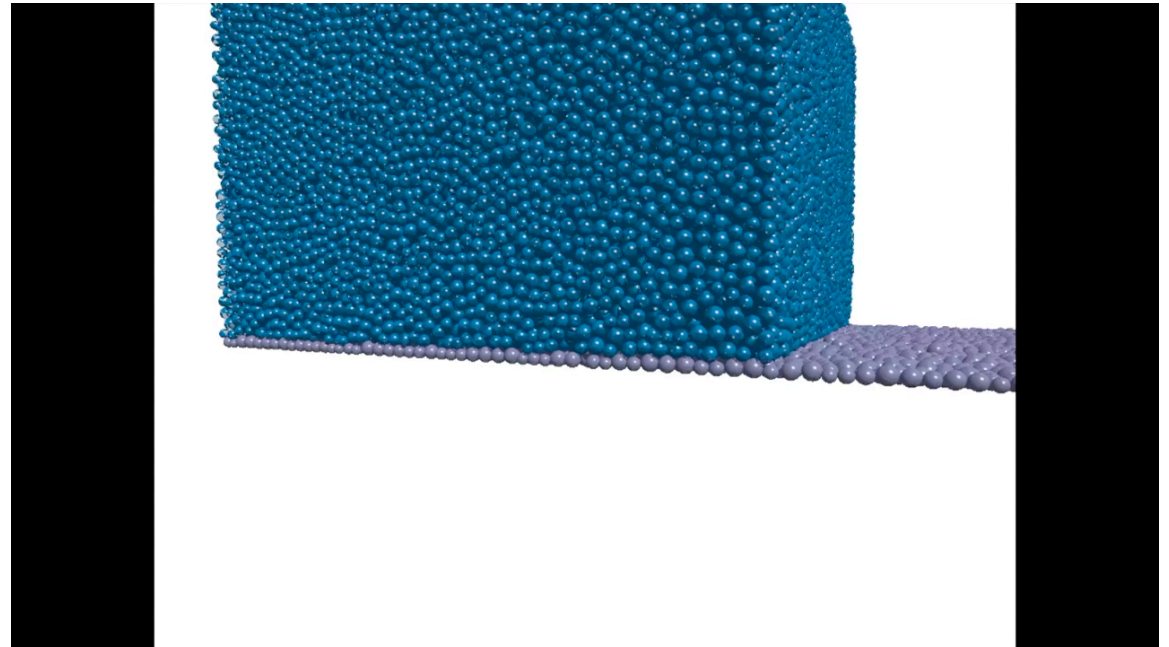


Numerical tests.

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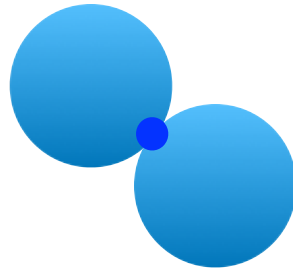


▶ 2D simulation - 70 000 spheres



▶ 3D simulation - 112 000 spheres

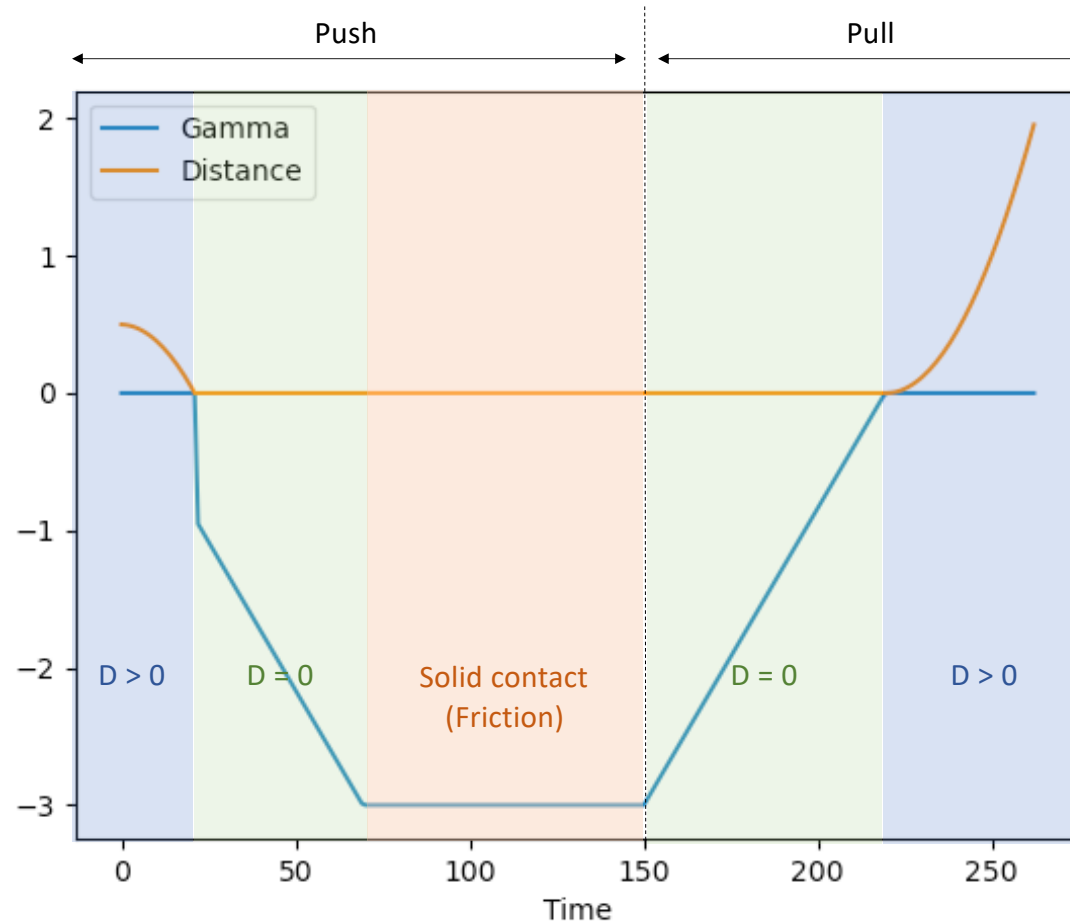
Contact law



Gluey contacts
Inelastic collisions
Coulomb friction law

[PhD Quentin Houssier]

Coupling lubrication and friction.



Coupling lubrication and friction.

Discrete energy
[reminder]

► Gluey contact

$$(\lambda_+, \lambda_-) \in F = \mathbb{R}^+ \times \mathbb{R}^+$$

$$E(\mu_+, \mu_-) = (\mu_+ - \mu_-) \left(q^k + \Delta t \frac{u_\mu + \bar{u}^{k+1}}{2} \right)$$

► Friction

$$\boldsymbol{\lambda} \in \mathbf{F} = \{ \boldsymbol{\mu} = \mu_n \mathbf{n} + \boldsymbol{\mu}_t \in \mathbb{R}^3 / |\boldsymbol{\mu}_t| \leq \mu \mu_n \}$$

$$E(\boldsymbol{\mu}) = \mu_n \left[D^k + \Delta t \mathbf{n} \cdot A^k \left(\frac{\mathbf{u}_\mu + \bar{\mathbf{u}}^{k+1}}{2} \right) \right] \\ + \boldsymbol{\mu}_t \cdot \left[\Delta t \mathbf{T}^k A^k \left(\frac{\mathbf{u}_\mu + \bar{\mathbf{u}}^{k+1}}{2} \right) \right]$$

Coupling lubrication and friction.

Discrete energy

► Gluey contact and friction

$$(\boldsymbol{\lambda}, \lambda_-) \in \mathbf{F}$$

$$\mathbf{F} = \{(\boldsymbol{\mu}, \mu_-) = (\mu_n \mathbf{n} + \boldsymbol{\mu}_t, \mu_-) \in \mathbb{R}^3 \times \mathbb{R} / \mu_- \geq 0, |\boldsymbol{\mu}_t| \leq \mu \mu_n, \mu_- \mu_n = 0\}$$

$$E(\boldsymbol{\mu}) = (\mu_n - \mu_-) \left[D^k + \Delta t \mathbf{n} \cdot A^k \left(\frac{\mathbf{u}_\mu + \bar{\mathbf{u}}^{k+1}}{2} \right) \right] + \boldsymbol{\mu}_t \cdot \left[\Delta t \mathbf{T}^k A^k \left(\frac{\mathbf{u}_\mu + \bar{\mathbf{u}}^{k+1}}{2} \right) \right]$$

Coupling lubrication and friction.

Discrete energy

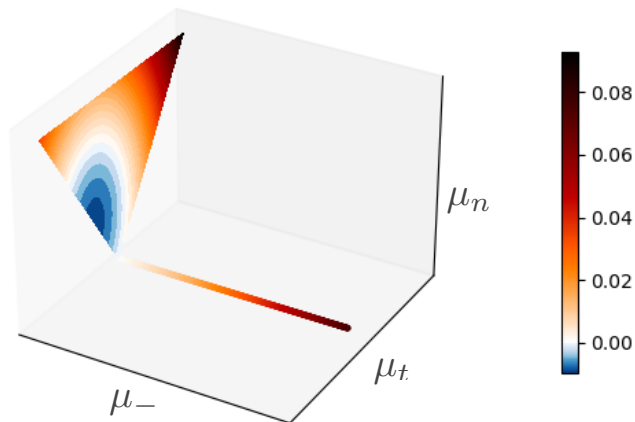
► Gluey contact and friction

$$(\lambda, \lambda_-) \in \mathbf{F}$$

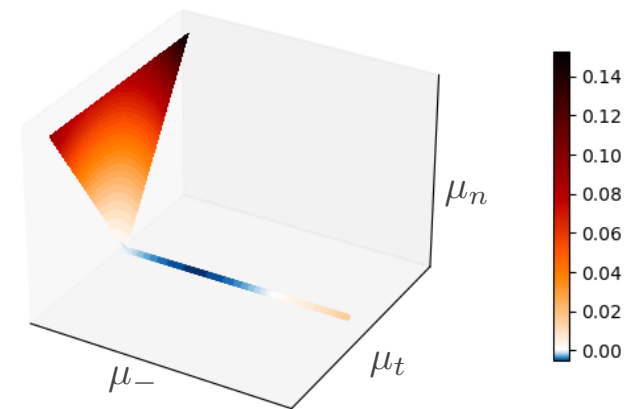
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Non convex

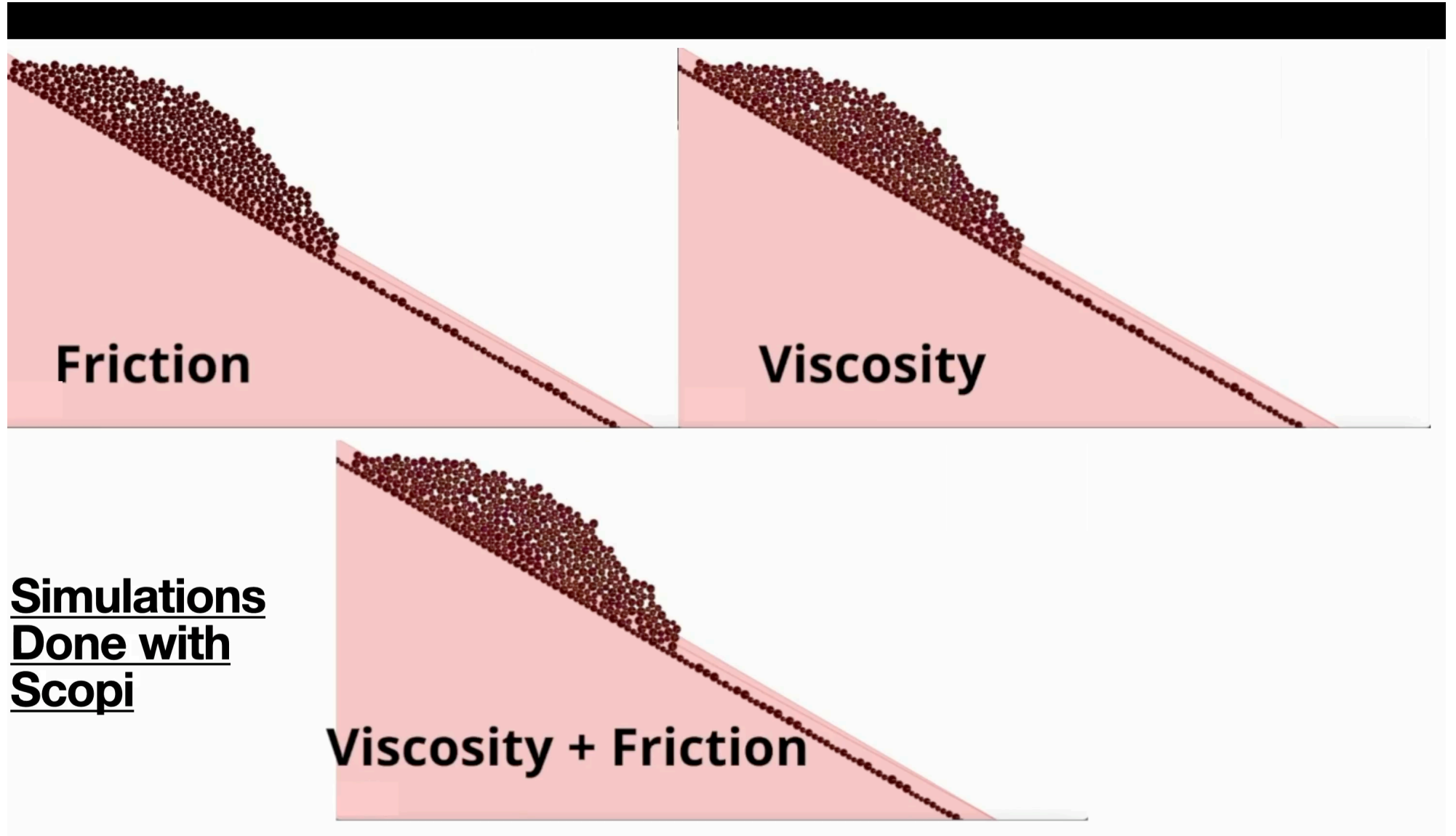


Push: activate friction



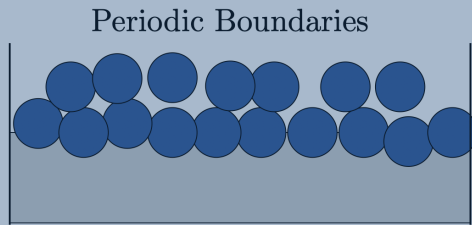
Pull: activate lubrication

Numerical tests

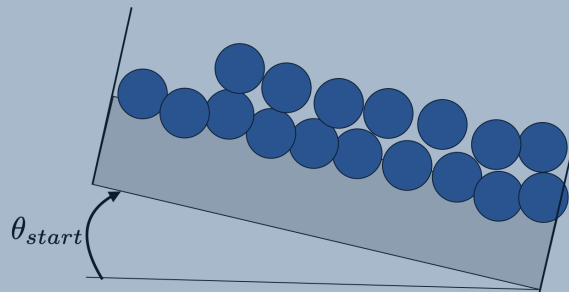


Numerical experiment: avalanche angle

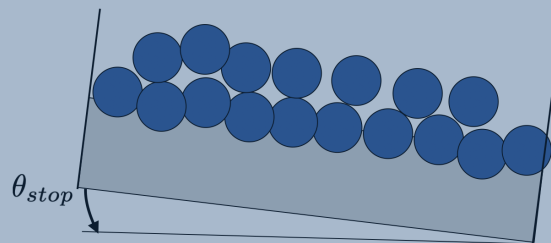
▶ Step 1



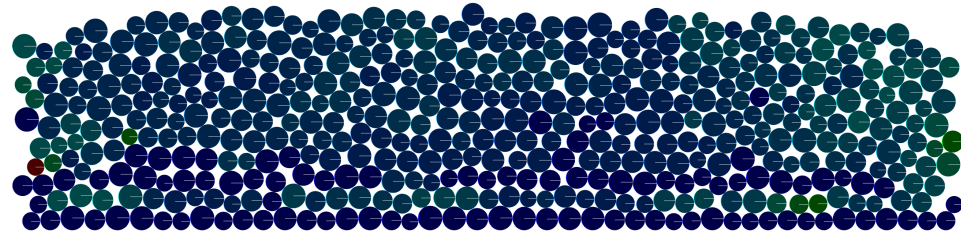
▶ Step 2



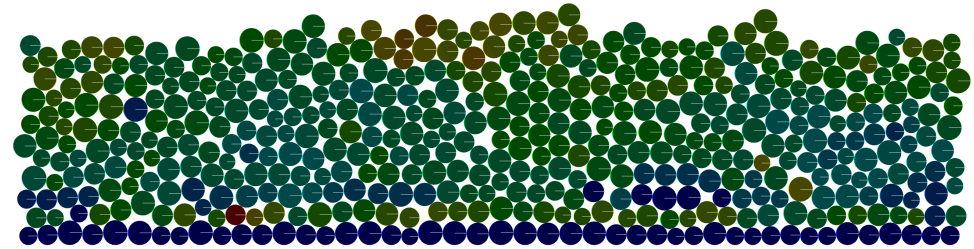
▶ Step 3



▶ Lubrication, No friction, $\theta = 8^\circ$, no flow



▶ Lubrication, No friction, $\theta = 12^\circ$, flowing



	θ_{start}	θ_{stop}
No friction	12	11
Friction	17	12

[with B. Darbois-Textier, G. Gauthier, FAST]

Prospects.

- ▶ Understand the « projection » on the non convex set
- ▶ Convergence study of the different schemes
- ▶ Modelling
 - ▶ Include elastic collisions
- ▶ Avalanche angle experiment:
 - ▶ Local stress, Coordination number
 - ▶ Influence of inertia
- ▶ Soils: Consider fibers, living beings
- ▶ Add various local forces (cohesion, repulsion, shear-thickening)
- ▶ Taking lubrication effect and solid collision in macroscopic PDE models for granular flows (with Charlotte Perrin)

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